

Energy of One-Dimensional Diatomic Elastic Granular Gas: Theory and Molecular Dynamics Simulation

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Abstract

One-dimensional ideal diatomic gas is simulated through possible types of motions of its molecule. Energy of each type of its motion is calculated by both theoretical and numerical methods. Analytical calculation of kinetic energy of an atom in translational-vibrational motion is not simple, but it can be solved by numerical method using molecular dynamic simulation. This paper justifies that the kinetic energy of a diatomic molecule can be determined by two different approaches which give the same results. In the first approach, the kinetic energy is calculated as a summation of kinetic energy of each atom. In the second approach, the kinetic energy is calculated as a summation of kinetic energy of translational and vibrational motions.

Keywords: One-dimension; Granular gas; Diatomic molecule; Simulation.

1. Introduction

Motion of diatomic gas molecules, which is temperature dependent, is contributed from three types of motion: translational, rotational, and vibrational. It is already obvious to consider that those types of motion are independent, which lead to the well known concept of equipartition energy and degree of freedom. This concept has been theoretically established^{1,2}. Students generally do not realize that a diatomic molecule may make a motion contains more than one type of motion, as we have been observed recently. Therefore, it is required to build a model of motion of a diatomic molecule in order to connect between that abstract concept and students' concrete understanding.

One way to model the motion of gas molecules is to use a simulated granular material. An atom is modeled as a ball. One method that is commonly used is the soft-sphere³ using molecular dynamics method implemented Gear predictor-corrector algorithm⁴. As a first step, the problem is limited to one-dimensional case. There is a study on collision properties⁵ and energy transport⁶, free cooling⁷, and kinetic description⁸ of one-dimensional granular gas. One-dimensional ideal diatomic gas which is simulated through motion of a molecule in order to observe its possible types of motion is reported in this work. Energy calculation from theory and numerical method is also discussed.

2. Theoretical Background

This paper discusses a one-dimensional ideal diatomic gas so that there are no friction and no van der Waals forces. The gas is kept at constant temperature. A diatomic gas molecule is modeled as two atoms which are connected by an ideal spring to relate the inter-atomic bonding. For one-dimensional

motion, the molecule is moving with its trajectories are straight lines. A molecule can move translational, vibrational, or translational-vibrational. The energy of this molecule is discussed by reviewing the kinetic energy and potential energy separately.

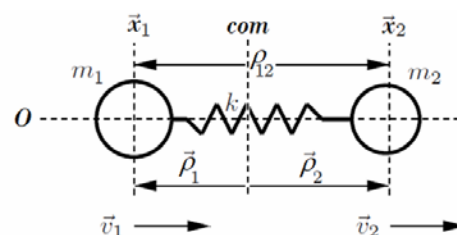


Figure 1. A model of a diatomic molecule as two atoms connected by an ideal spring.

Mass, position, velocity, momentum and kinetic energy of the i th atom are denoted by $m_i, \vec{x}_i, \vec{v}_i, \vec{p}_i$ and K_i . Index s denotes for system of a diatomic molecule. Kinetic energy of the system is

$$K_s = K_1 + K_2 = \frac{1}{2} m_1 v_1^2 + \frac{1}{2} m_2 v_2^2 = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} \quad (1)$$

If a diatomic molecule is treated as a point, coordinate and momentum of this point correspond to the center of mass (com) of the molecule so that there are two groups of variables. The first is related to the center of mass, while the latter to internal system denoted by Greek symbol. Kinetic energy of the system is then written as⁹:

$$K_s = \frac{p_s^2}{2m_s} + \frac{1}{2} \mu \dot{\rho}_{12}^2 \quad (2)$$

where μ is the reduced mass of the system

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \quad (3)$$

ρ_{12} is distance between the two atoms and $\dot{\rho}_{12}$ is its time derivative.

$$\bar{\rho}_{12} = \bar{\rho}_1 - \bar{\rho}_2 = \bar{x}_1 - \bar{x}_2 = \bar{x}_{12} \quad (4)$$

If the spring between two atoms in the system has spring constant k then potential energy of the system is

$$U = \frac{1}{2} k (\rho_0 - \rho_{12})^2 \quad (5)$$

where ρ_0 is an equilibrium distance.

The energy of the molecule is

$$E = K_s + U = \left(\frac{1}{2} m_1 v_1^2 + \frac{1}{2} m_2 v_2^2 \right) + \frac{1}{2} k (\rho_0 - \rho_{12})^2 \quad (6)$$

or

$$E = E_{trans} + E_{vib} = \left(\frac{p_s^2}{2m_s} \right) + \left[\frac{1}{2} \mu \dot{\rho}_{12}^2 + \frac{1}{2} k (\rho_0 - \rho_{12})^2 \right] \quad (7)$$

3. Simulation Procedure

Two grains which are connected with an ideal spring are used to simulate a diatomic molecule. The spring force \bar{S}_{ij} between the two grains is:

$$\bar{S}_{ij} = k(\rho_0 - \rho_{ij})\hat{\rho}_{ij} - \gamma \bar{v}_{ij} \quad (8)$$

γ is a constant called damping coefficient and the role of $-\gamma \bar{v}_{ij}$ is a dissipative force.

Period of vibrational motion is

$$\tau_{vib} = 2\pi \sqrt{\frac{\mu}{k}} \quad (9)$$

Gear predictor-corrector algorithm of fifth order⁴⁾ is chosen in the molecular dynamics method used in the simulation, which has two steps: prediction step (written with upper index p) and correction step for every particular grain. The first step is formulated as

$$\begin{pmatrix} \bar{r}_0^p(t+\Delta t) \\ \bar{r}_1^p(t+\Delta t) \\ \bar{r}_2^p(t+\Delta t) \\ \bar{r}_3^p(t+\Delta t) \\ \bar{r}_4^p(t+\Delta t) \\ \bar{r}_5^p(t+\Delta t) \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 & 4 & 5 \\ 0 & 0 & 1 & 3 & 6 & 10 \\ 0 & 0 & 0 & 1 & 4 & 10 \\ 0 & 0 & 0 & 0 & 1 & 5 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \bar{r}_0(t) \\ \bar{r}_1(t) \\ \bar{r}_2(t) \\ \bar{r}_3(t) \\ \bar{r}_4(t) \\ \bar{r}_5(t) \end{pmatrix} \quad (10)$$

And the correction step will give the corrected value of $\bar{r}_n(t+\Delta t)$ through

$$\begin{pmatrix} \bar{r}_0(t+\Delta t) \\ \bar{r}_1(t+\Delta t) \\ \bar{r}_2(t+\Delta t) \\ \bar{r}_3(t+\Delta t) \\ \bar{r}_4(t+\Delta t) \\ \bar{r}_5(t+\Delta t) \end{pmatrix} = \begin{pmatrix} \bar{r}_0^p(t+\Delta t) \\ \bar{r}_1^p(t+\Delta t) \\ \bar{r}_2^p(t+\Delta t) \\ \bar{r}_3^p(t+\Delta t) \\ \bar{r}_4^p(t+\Delta t) \\ \bar{r}_5^p(t+\Delta t) \end{pmatrix} + \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{pmatrix} \Delta \bar{r}_2(t+\Delta t), \quad (11)$$

with

$$\Delta \bar{r}_2(t+\Delta t) = \bar{r}_2(t+\Delta t) - \bar{r}_2^p(t+\Delta t) \quad (12)$$

The term $\bar{r}_n(t+\Delta t)$ is defined as

$$\bar{r}_n(t) = \frac{(\Delta t)^n}{n!} \left[\frac{d^n \bar{r}_0(t)}{dt^n} \right], \quad (13)$$

where \bar{r}_0 is position of a grain. The term $\bar{r}_2(t+\Delta t)$ in correction term in Equation (12) is obtained from Newton's second law of motion. For example, particle i has

$$[\bar{r}_2(t+\Delta t)]_i = \frac{(\Delta t)^2}{m_i} \sum_{j \neq i} \bar{S}_{ij}(t+\Delta t). \quad (14)$$

The left part of Equation (11) is calculated using $\bar{r}_n^p(t+\Delta t)$.

4. Results and Discussion

4.1 Kinetic, potential, and mechanical energies

A simulation result for a diatomic molecule in translational, vibrational, and translational-vibrational motions are given in Figure 2. Position of the two atoms as a function of time is shown for each case. Simulation parameters are $m_1 = m_2 = 2$, $k = 100$, and $\gamma = 0$. The two atoms are initially at $\bar{x}_1(t=0) = -0.5$ and $\bar{x}_2(t=0) = 0.5$ so that its equilibrium distance $\rho_0 = 1.0$.

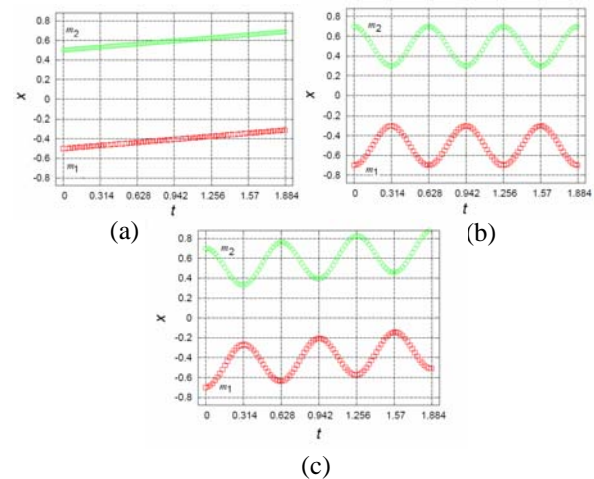


Figure 2. Position-time graph for the two atoms of a molecule: (a) translational, (b) vibrational, and (c) translational-vibrational motion.

The translational velocity of the atoms in Figure 2(a) is $\vec{v}_1 = \vec{v}_2 = 0.1$ so that the distance between the atoms is constant ($\rho_{12} = \rho_0 = 1.0$) and its time derivative is zero ($\dot{\rho}_{12} = \dot{v}_{12} = 0$). Kinetic, potential, and total energies for this translational motion are

$$K_{trans} = \frac{1}{2}m_1v_1^2 + \frac{1}{2}m_2v_2^2 = 0.01 + 0.01 = 0.02 \quad (15)$$

$$U_{trans} = \frac{1}{2}k(\rho_0 - \rho_{12})^2 = 0 \quad (16)$$

$$E_{trans} = K_{trans} + U_{trans} = 0.02 \quad (17)$$

In Figure 2(b) each atom is deflected outward 0.2 from their initial positions so that molecule vibrates with amplitude $A = 0.4$ at period $\tau_{vib} = 0.2\pi$. The distance between the two atoms from its equilibrium changes with time in sinusoidal function.

$$(\rho_{ij} - \rho_0) = A \cos(\omega_{vib}t)$$

Its relative velocity between the two atoms is also in sinusoidal function.

$$\dot{\rho}_{ij} = -A\omega_{vib} \sin(\omega_{vib}t)$$

For this vibrational motion, position of the center of mass is fixed ($\vec{v}_s = 0$ and $\vec{p}_s = 0$). Kinetic, potential, and total energies for this vibrational motion are

$$\begin{aligned} K_{vib} &= \frac{1}{2}\mu(\dot{\rho}_{12})^2 \\ &= \frac{1}{2}\mu(-A\omega_{vib} \sin(\omega_{vib}t))^2 \\ &= \frac{1}{2}kA^2 \sin^2(\omega t) \\ &= 8\sin^2(10t) \end{aligned} \quad (18)$$

$$\begin{aligned} U_{vib} &= \frac{1}{2}k(\rho_{12} - \rho_0)^2 \\ &= \frac{1}{2}kA^2 \cos^2(\omega_{vib}t) \\ &= 8\cos^2(10t) \end{aligned} \quad (19)$$

$$E_{vib} = K_{vib} + U_{vib} = \frac{1}{2}kA^2 = 8 \quad (20)$$

Figure 2(c) shows translational-vibrational motion. Kinetic, potential, and total energies for this motion are

$$\begin{aligned} K &= \frac{p_s^2}{2m_s} + \frac{1}{2}\mu(\dot{\rho}_{12})^2 \\ &= \frac{1}{2}m_s v_s^2 + \frac{1}{2}\mu(-A\omega_{vib} \sin(\omega_{vib}t))^2 \\ &= 0.02 + \frac{1}{2}kA^2 \sin^2(\omega_{vib}t) \\ &= 0.02 + 8\sin^2(10t) \end{aligned} \quad (21)$$

$$\begin{aligned} U &= \frac{1}{2}k(\rho_{12} - \rho_0)^2 \\ &= \frac{1}{2}kA^2 \cos^2(\omega_{vib}t) = 8\cos^2(10t) \end{aligned} \quad (22)$$

$$E = K + U = 8.02 \quad (23)$$

4.2 Kinetic energy

For translational-vibrational motion shown in Figure 2(c), its kinetic energy of the diatomic molecule is calculated using two different ways. First, kinetic energy is determined from each atom based on equation (1) as shown in Figure 3(a). Second, kinetic energy is determined from translational and vibrational motion separately based on equation (2) as shown in Figure 3(b).

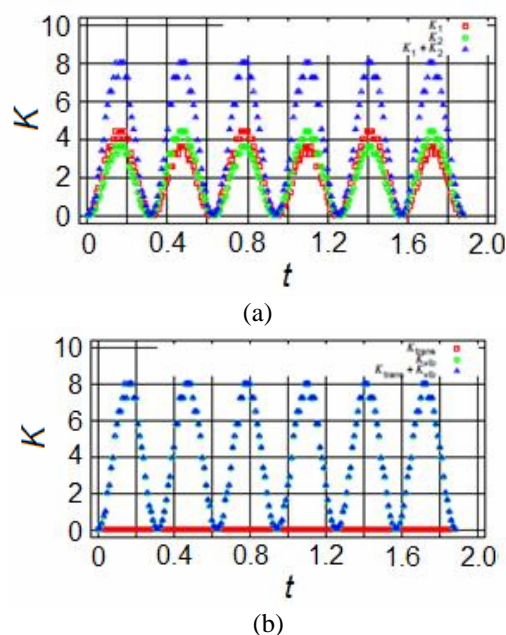


Figure 3. Kinetic energy-time graph for molecule motion in Figure 2(c): (a) kinetic energy of each atom (b) kinetic energy for translational and vibrational motions separately.

Calculation of kinetic energy of an atom moving in translational-vibrational motion is not analytically simple, since it is not easy to express its mathematical function of its motion. However, it will be possible to determine its kinetic energy with the numerical method of molecular dynamic (Figure 3(a)). It can be seen from Figure 2(c) that its maximum magnitude of tangent (maximum speed) of m_1 in time interval 0 and 0.314 is at $t = 0.57$ and this maximum speed is slightly greater than that at $t = 0.471$ in time interval 0.314 and 0.628. It can also be observed that the maximum speed of m_2 is slightly greater than that of m_1 at time interval 0 and 0.314. Therefore, the maximum kinetic energy of m_1 is not exactly the same as m_2 and their values change alternately with time (Figure 3(a)).

Kinetic energy from translational motion and vibrational motion has been calculated in equations (15) and (18) respectively and its total is in equation

(21). Since K_{trans} is small compared to K_{vib} then the total is nearly the same as K_{vib} (Figure 3(b)).

Other phenomenon that is also interesting in gas is thermal transport. To study this property, temperature of the gas must be varied with time or position. On the other hand, the influence of electron distribution among atoms in a diatomic molecule can also be investigated by defining Hamiltonian for the system. Those two topics could be themes for further study.

5. Conclusion

Motion of a diatomic molecule has been simulated using granular particles. For one-dimensional ideal gas, kinetic energy of a diatomic molecule can be calculated as a total of kinetic energy from each atom or a total of kinetic energy from translational motion and vibrational motion. Calculation of kinetic energy of each atom can be solved by numerical method using molecular dynamic simulation.

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